

10/521,728B Yong chu 09-05-2007

\$%^STN;HighlightOn=;HighlightOff=;

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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	MAY 01	New CAS web site launched
NEWS	3	MAY 08	CA/Caplus Indian patent publication number format defined
NEWS	4	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS	5	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS	6	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS	7	MAY 21	CA/Caplus enhanced with additional kind codes for German patents
NEWS	8	MAY 22	CA/Caplus enhanced with IPC reclassification in Japanese patents
NEWS	9	JUN 27	CA/Caplus enhanced with pre-1967 CAS Registry Numbers
NEWS	10	JUN 29	STN Viewer now available
NEWS	11	JUN 29	STN Express, Version 8.2, now available
NEWS	12	JUL 02	LEMBASE coverage updated
NEWS	13	JUL 02	LMEDLINE coverage updated
NEWS	14	JUL 02	SCISEARCH enhanced with complete author names
NEWS	15	JUL 02	CHEMCATS accession numbers revised
NEWS	16	JUL 02	CA/Caplus enhanced with utility model patents from China
NEWS	17	JUL 16	Caplus enhanced with French and German abstracts
NEWS	18	JUL 18	CA/Caplus patent coverage enhanced
NEWS	19	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS	20	JUL 30	USGENE now available on STN
NEWS	21	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	22	AUG 06	BEILSTEIN updated with new compounds
NEWS	23	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	24	AUG 13	CA/Caplus enhanced with additional kind codes for granted patents
NEWS	25	AUG 20	CA/Caplus enhanced with CAS indexing in pre-1907 records
NEWS	26	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	27	AUG 27	USPATOLD now available on STN
NEWS	28	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 13:33:33 ON 05 SEP 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:33:54 ON 05 SEP 2007

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STRUCTURE FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2

DICTIONARY FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

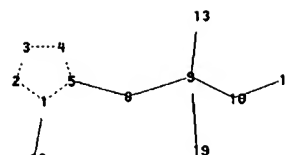
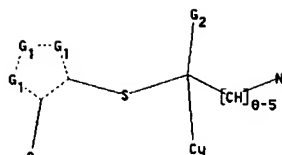
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728Q.str



chain nodes :
 8 9 10 11 13 16 19
 ring nodes :
 1 2 3 4 5
 chain bonds :
 1-16 5-8 8-9 9-10 9-13 9-19 10-11
 ring bonds :
 1-2 1-5 2-3 3-4 4-5
 exact/norm bonds :
 1-2 1-5 1-16 2-3 3-4 4-5 5-8 8-9 9-10 9-13 9-19 10-11

G1:C,S

G2:H,CH3,Et,n-Pr,n-Bu

G3:X,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 8:CLASS 9:CLASS 10:CLASS 11:CLASS
 13:CLASS
 16:CLASS 19:Atom
 Generic attributes :
 19:
 Saturation : Unsaturated
 Number of Carbon Atoms : less than 7

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 13:34:26 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 5668 TO ITERATE

35.3% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 108846 TO 117874
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 13:34:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 112533 TO ITERATE

100.0% PROCESSED 112533 ITERATIONS
SEARCH TIME: 00.00.06

7 ANSWERS

L3 7 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
172.55	172.76

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 13:35:02 ON 05 SEP 2007
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FILE COVERS 1907 - 5 Sep 2007 VOL 147 ISS 11
FILE LAST UPDATED: 4 Sep 2007 (20070904/ED)

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L4 2 L3

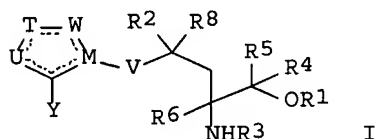
Not ODP.

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80678 CAPLUS Full-text
DOCUMENT NUMBER: 140:145993
TITLE: Preparation of aminohydroxyalkylthiothiophenecarbonitriles as nitric oxide synthase (NOS) inhibitors.

INVENTOR(S): Mete, Antonio; Walters, Iain
 PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.
 SOURCE: PCT Int. Appl., 37 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009580	A1	20040129	WO 2003-SE1215	20030715
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003245230	A1	20040209	AU 2003-245230	20030715
EP 1539731	A1	20050615	EP 2003-738863	20030715
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006504655	T	20060209	JP 2004-522890	20030715
US 2005203172	A1	20050915	US 2005-521727	20050118
PRIORITY APPLN. INFO.:			SE 2002-2279	A 20020719
			WO 2003-SE1215	W 20030715
OTHER SOURCE(S):		MARPAT 140:145993		
GI				



AB Title compds. [I; Y = (fluoro)alkyl, (fluoro)alkoxy, halo, CN, C:CH, NO₂, CH₂OH, CHO, Ac, NH₂, NHCHO, NHCOCH₃, NHSO₂Me; T, U, W = CX, N, NR₁₃, O, SOm; m = 0-2; X = H, (fluoro)alkyl, (fluoro)alkoxy, halo, OH, SH, CN, C:CH, N(R₁₄)₂, NO₂, CH₂OH, CHO, Ac, NHCHO; V = NR₇, O, CH₂, SOn, CH₂O, CH₂NR₇, CH₂SOn, CH₂CH₂, CH:CH; n = 0-2; M = C, N; R₁, R₈ = H, Me.; R₂ = alkyl, alkenyl, alkynyl, cycloalkyl, 4-8 membered satd. heterocyclyl incorporating 1 O, S, N; any of said groups being optionally further substituted by alkyl, alkoxy, alkylthio, cycloalkyl, halo, (substituted) Ph; or R₂ = (substituted) Ph, 5-6 membered heteroaryl contg. 1-3 O, S, N; R₃ = H, (substituted) alkyl, cycloalkyl; R₄-R₇, R₉-R₁₂, R₁₄ = H, alkyl; R₁₃ = H, alkyl, CHO, Ac, SO₂CH₃, CF₃], were prepd. Thus, 1,1-dimethylethyl (4S)-4-((2R)-2-mercapto-2-phenylethyl)-2,2-dimethyl-3-oxazolidinecarboxylate (prepn. given), 3-bromothiophene-2-carbonitrile, and NaH were stirred 24 h in DMF to give 1,1-dimethylethyl (4S)-4-[(2R)-2-[(2-cyano-3-thienyl)thio]-2-phenylethyl]-2,2-dimethyl-3-oxazolidinecarboxylate. The latter was stirred 2 h with 4M HCl in dioxane to give a residue which was treated with oxalic acid in Et₂O to give

3-[[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-2-thiophenecarbonitrile oxalate. I inhibited iNOS with IC50 <10 .mu.M.

IT 651353-83-2P 651353-84-3P 651353-85-4P
651353-86-5P

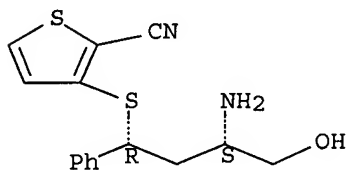
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aminohydroxyalkylthiothiophenecarbonitriles as nitric oxide synthase inhibitors)

RN 651353-83-2 CAPLUS

CN 2-Thiophenecarbonitrile, 3-[[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-(9CI) (CA INDEX NAME)

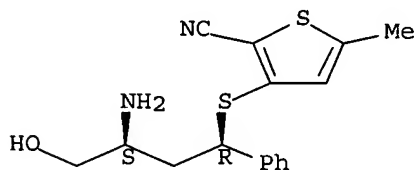
Absolute stereochemistry.



RN 651353-84-3 CAPLUS

CN 2-Thiophenecarbonitrile, 3-[[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 651353-85-4 CAPLUS

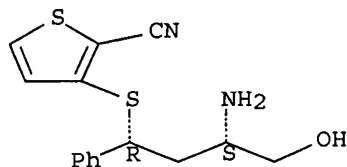
CN 2-Thiophenecarbonitrile, 3-[[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 651353-83-2

CMF C15 H16 N2 O S2

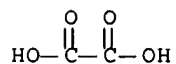
Absolute stereochemistry.



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 651353-86-5 CAPLUS

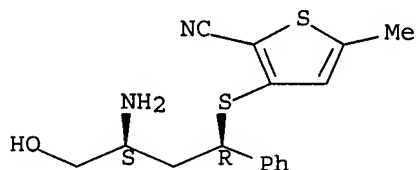
CN 2-Thiophenecarbonitrile, 3-[[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-5-methyl-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 651353-84-3

CMF C16 H18 N2 O S2

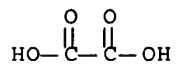
Absolute stereochemistry.



CM 2

CRN 144-62-7

CMF C2 H2 O4



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

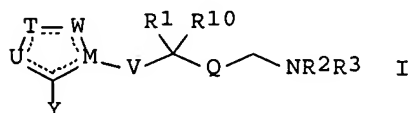
L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80677 CAPLUS Full-text

DOCUMENT NUMBER: 140:128265

TITLE: Preparation of 3-[[[(1S)-2-amino-1-phenylethyl]thio]-5-methyl-2-thiophenecarbonitrile oxalate and related compounds as nitric oxide synthase inhibitors.

INVENTOR(S): Mete, Antonio; Walters, Iain
 PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.
 SOURCE: PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009579	A1	20040129	WO 2003-SE1214	20030715
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003251259	A1	20040209	AU 2003-251259	20030715
EP 1539732	A1	20050615	EP 2003-765417	20030715
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005537281	T	20051208	JP 2004-522889	20030715
US 2006019999	A1	20060126	US 2005-521728	20050118
PRIORITY APPLN. INFO.:			SE 2002-2280	A 20020719
			WO 2003-SE1214	W 20030715
OTHER SOURCE(S):		MARPAT 140:128265		
GI				



AB Title compds. [I; Y = (F-substituted) alkyl, alkoxy, halo, CN, C:CH, NO₂, CH₂OH, CHO, Ac, NH₂, NHCHO, NHAc, NHSO₂Me; T, U, W = CX, N, NR₉, O, S(O)_m, .gtoreq.1 of T, U, W must = heteroatom and .ltoreq.1 of T, U and W may = NR₉, O, SO_m; m, n = 0-2; X = H, (F-substituted) alkyl, alkoxy, halo, OH, SH, CN, C:CH, N(R₁₁)₂, NO₂, CH₂OH, CHO, Ac, NHCHO; V = NR₄, O, CH₂, SO_n, OCH₂, CH₂O, NR₄CH₂, CH₂NR₄, CH₂SO_n, SO_nCH₂, CH₂CH₂, CH:CH; M = C, and when M is bonded to a CH₂ moiety in V, then M may = N; R₁₀ = H, Me. Q = (CH₂)_p; p = 0-3; R₁ = (substituted) Ph, 5-6 membered heteroaryl contg. 1-3 O, S and N; R₂, R₃ = H, (substituted) alkyl, cycloalkyl; Z = CO, bond; R₄, R₁₁ = H, alkyl; R₅-R₈ = H, alkyl; R₉ = H, alkyl, CHO, Ac, SO₂Me, CF₃], were prepd. Thus, S-[(1S)-2-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-phenylethyl]benzenecarbothioate (prepn. given) was stirred 2h with aq. NH₃ in MeOH; the residue was stirred with 3-bromo-5-methyl-2-thiophenecarbonitrile (prepn. given) and Cs₂CO₃ in DMF for 24 h to give 1,1-dimethylethyl [(2S)-2-[(2-cyano-5-methyl-3-thienyl)thio]-2-phenylethyl]carbamate. The latter was stirred with 4M HCl in dioxane at 20.degree. for 2 h and the residue was treated with oxalic acid in Et₂O to give 3-[(1S)-2-amino-1-phenylethylthio]-5-methyl-2-

thiophenecarbonitrile oxalate. The latter inhibited nitric oxide synthase with IC50 <100 .mu.M.

IT 651034-24-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aminophenylethylthiomethylthiophenecarbonitrile and related compds. as nitric oxide synthase inhibitors)

RN 651034-24-1 CAPLUS

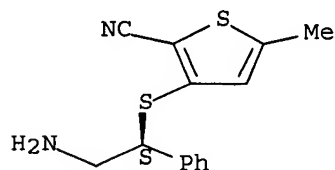
CN 2-Thiophenecarbonitrile, 3-[[[(1S)-2-amino-1-phenylethyl]thio]-5-methyl-, ethanedioate (9CI) (CA INDEX NAME)

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CRN 651034-23-0

CMF C14 H14 N2 S2

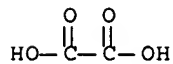
Absolute stereochemistry.



CM 2

CRN 144-62-7

CMF C2 H2 O4



IT 651034-45-6P

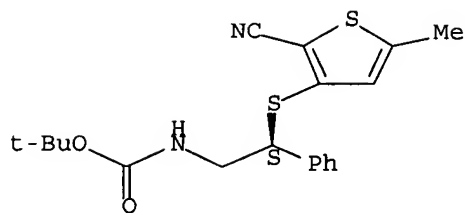
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of aminophenylethylthiomethylthiophenecarbonitrile and related compds. as nitric oxide synthase inhibitors)

RN 651034-45-6 CAPLUS

CN Carbamic acid, [(2S)-2-[(2-cyano-5-methyl-3-thienyl)thio]-2-phenylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
21.82	194.58

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.56	-1.56

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 13:49:26 ON 05 SEP 2007

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STRUCTURE FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2

DICTIONARY FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

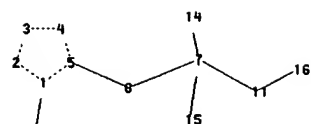
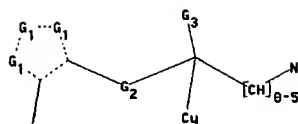
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728R.str



chain nodes :

6 7 8 11 14 15 16

ring nodes :

1 2 3 4 5

chain bonds :

1-8 5-6 6-7 7-11 7-14 7-15 11-16

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-11 7-14 7-15 11-16

G1:C,S

G2:O,S,N,CH2

G3:H,CH3,Et,n-Pr,n-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:Atom

14:CLASS

15:Atom 16:CLASS

Generic attributes :

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Saturation : Unsaturated

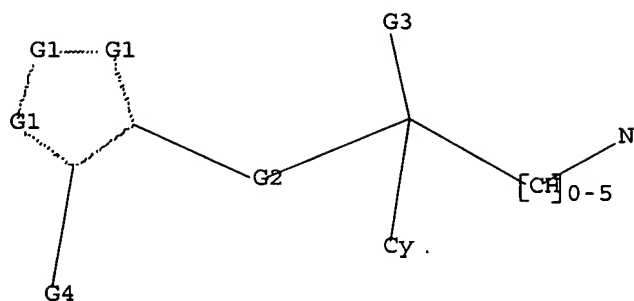
Number of Carbon Atoms : less than 7

L5 STRUCTURE UPLOADED

=> d

L5 HAS NO ANSWERS

L5 STR



G1 C, S
 G2 O, S, N, CH2
 G3 H, Me, Et, n-Pr, n-Bu
 G4 X, MeO, EtO, n-PrO, i-PrO, n-BuO, s-BuO, CN, CHO, NH, NH2, NO2

Structure attributes must be viewed using STN Express query preparation.

=> s 15
 SAMPLE SEARCH INITIATED 13:49:56 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 735141 TO ITERATE

0.3% PROCESSED 2000 ITERATIONS 0 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.04

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**
 PROJECTED ITERATIONS: 14655654 TO 14749986
 PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 full
 FULL SEARCH INITIATED 13:50:34 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 14703568 TO ITERATE

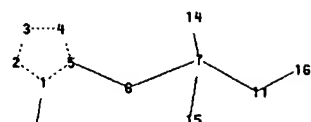
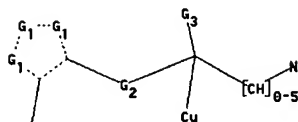
1.9% PROCESSED 272888 ITERATIONS 0 ANSWERS
 3.7% PROCESSED 548769 ITERATIONS 0 ANSWERS
 5.1% PROCESSED 745208 ITERATIONS 0 ANSWERS
 6.6% PROCESSED 973220 ITERATIONS 0 ANSWERS
 6.8% PROCESSED 1000000 ITERATIONS 0 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.01.12

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**
 PROJECTED ITERATIONS: 14703568 TO 14703568
 PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS FUL L5

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728R-1.str



chain nodes :

6 7 8 11 14 15 16

ring nodes :

1 2 3 4 5

chain bonds :

1-8 5-6 6-7 7-11 7-14 7-15 11-16

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-11 7-14 7-15 11-16

G1:C,S

G2:O,N,CH2

G3:H,CH3,Et,n-Pr,n-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:Atom

14:CLASS

15:Atom 16:CLASS

Generic attributes :

15:

Saturation : Unsaturated

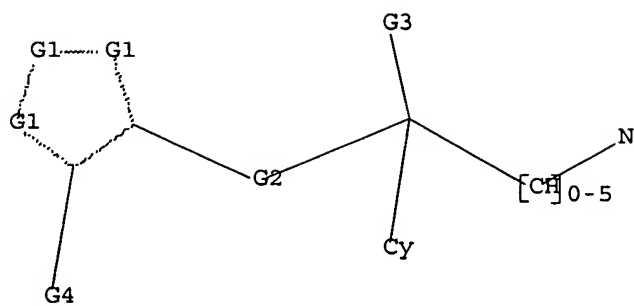
Number of Carbon Atoms : less than 7

L8 STRUCTURE UPLOADED

=> d

L8 HAS NO ANSWERS

L8 STR



G1 C, S
 G2 O, N, CH2
 G3 H, Me, Et, n-Pr, n-Bu
 G4 X, MeO, EtO, n-PrO, i-PrO, n-BuO, s-BuO, CN, CHO, NH, NH2, NO2

Structure attributes must be viewed using STN Express query preparation.

=> s 18

SAMPLE SEARCH INITIATED 13:53:23 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 722979 TO ITERATE

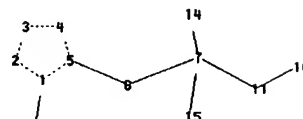
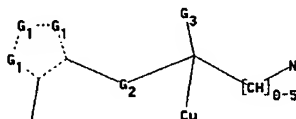
0.3% PROCESSED 2000 ITERATIONS 0 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.04

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**
 PROJECTED ITERATIONS: 14412733 TO 14506427
 PROJECTED ANSWERS: 0 TO 0

L9 0 SEA SSS SAM L8

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728R-2.str



chain nodes :
 6 7 8 11 14 15 16
 ring nodes :
 1 2 3 4 5
 chain bonds :
 1-8 5-6 6-7 7-11 7-14 7-15 11-16

ring bonds :
 1-2 1-5 2-3 3-4 4-5
 exact/norm bonds :
 1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-11 7-14 7-15 11-16

G1:C,S

G2:O,N

G3:H,CH3,Et,n-Pr,n-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:Atom
 14:CLASS

15:Atom 16:CLASS

Generic attributes :

15:

Saturation : Unsaturated

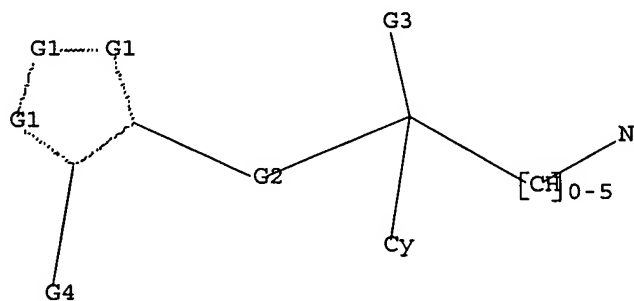
Number of Carbon Atoms : less than 7

L10 STRUCTURE UPLOADED

=> d

L10 HAS NO ANSWERS

L10 STR



G1 C,S

G2 O,N

G3 H,Me,Et,n-Pr,n-Bu

G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l10

SAMPLE SEARCH INITIATED 13:54:43 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 572155 TO ITERATE

0.3% PROCESSED 2000 ITERATIONS

0 ANSWERS

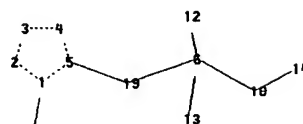
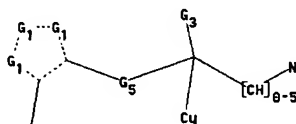
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 11400624 TO 11485576
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728R-3.str



chain nodes :

6 7 10 12 13 14 19

ring nodes :

1 2 3 4 5

chain bonds :

1-7 5-19 6-13 6-10 6-12 6-19 10-14

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-7 2-3 3-4 4-5 5-19 6-13 6-10 6-12 6-19 10-14

G1:C,S

G3:H,CH3,Et,n-Pr,n-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

G5:O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 10:Atom 12:CLASS

13:Atom

14:CLASS 19:CLASS

Generic attributes :

13:

Saturation : Unsaturated

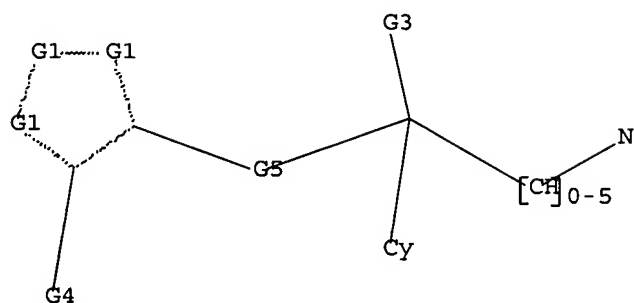
Number of Carbon Atoms : less than 7

L12 STRUCTURE UPLOADED

=> d

L12 HAS NO ANSWERS

L12 STR



G1 C, S

G2

G3 H, Me, Et, n-Pr, n-Bu

G4 X, MeO, EtO, n-PrO, i-PrO, n-BuO, s-BuO, CN, CHO, NH, NH2, NO2

G5 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s l12

SAMPLE SEARCH INITIATED 13:56:42 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 572155 TO ITERATE

0.3% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

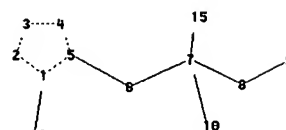
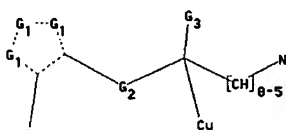
PROJECTED ITERATIONS: 11400624 TO 11485576

PROJECTED ANSWERS: 0 TO 0

L13 0 SEA SSS SAM L12

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728S.str



```

chain nodes :
6 7 8 9 10 15 20
ring nodes :
1 2 3 4 5
chain bonds :
1-20 5-6 6-7 7-8 7-10 7-15 8-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-20 2-3 3-4 4-5 5-6 6-7 7-8 7-10 7-15 8-9

```

G1:C,S

G2:O,N,CH2

G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom
15:CLASS 20:CLASS
Generic attributes :
10:
Saturation           : Unsaturated
Number of Carbon Atoms : less than 7

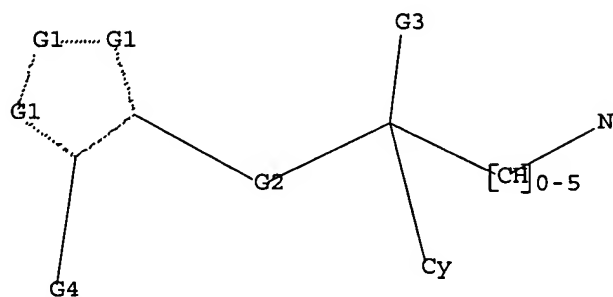
```

L14 STRUCTURE UPLOADED

=> d

L14 HAS NO ANSWERS

L14 STR



G1 C,S

G2 O,N,CH2

G3 H,Me,Et,n-Pr,i-Pr,n-Bu,s-Bu

G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l14

SAMPLE SEARCH INITIATED 14:00:56 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 722979 TO ITERATE

0.3% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.03

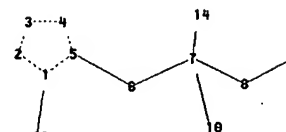
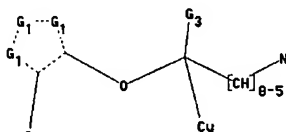
0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 14412733 TO 14506427
PROJECTED ANSWERS: 0 TO 0

L15 0 SEA SSS SAM L14

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728S-1.str



chain nodes :

6 7 8 9 10 14 19

ring nodes :

1 2 3 4 5

chain bonds :

1-19 5-6 6-7 7-8 7-10 7-14 8-9

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-19 2-3 3-4 4-5 5-6 6-7 7-8 7-10 7-14 8-9

G1:C,S

G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom
14:CLASS 19:CLASS

Generic attributes :

10:

Saturation : Unsaturated

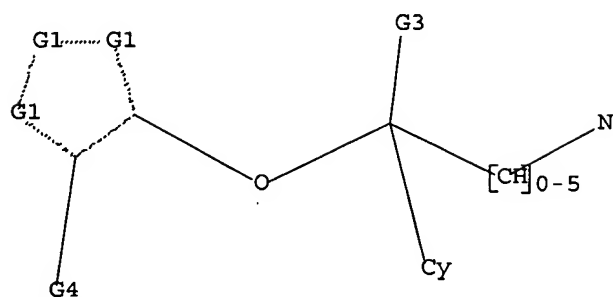
Number of Carbon Atoms : less than 7

L16 STRUCTURE UPLOADED

=> d

L16 HAS NO ANSWERS

L16 STR



G1 C, S

G2

G3 H, Me, Et, n-Pr, i-Pr, n-Bu, s-Bu

G4 X, MeO, EtO, n-PrO, i-PrO, n-BuO, s-BuO, CN, CHO, NH, NH2, NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l16

SAMPLE SEARCH INITIATED 14:02:23 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 30976 TO ITERATE

6.5% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 608996 TO 630044
PROJECTED ANSWERS: 0 TO 0

L17 0 SEA SSS SAM L16

=> s l16 full

FULL SEARCH INITIATED 14:02:32 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614816 TO ITERATE

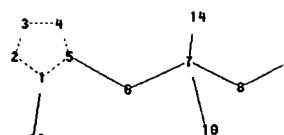
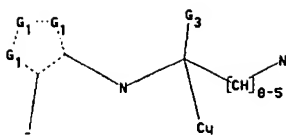
100.0% PROCESSED 614816 ITERATIONS
SEARCH TIME: 00.00.06

0 ANSWERS

L18 0 SEA SSS FUL L16

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728S-2.str



chain nodes :

6 7 8 9 10 14 19

ring nodes :

1 2 3 4 5

chain bonds :

1-19 5-6 6-7 7-8 7-10 7-14 8-9

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-19 2-3 3-4 4-5 5-6 6-7 7-8 7-10 7-14 8-9

G1:C,S

G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom

14:CLASS 19:CLASS

Generic attributes :

10:

Saturation : Unsaturated

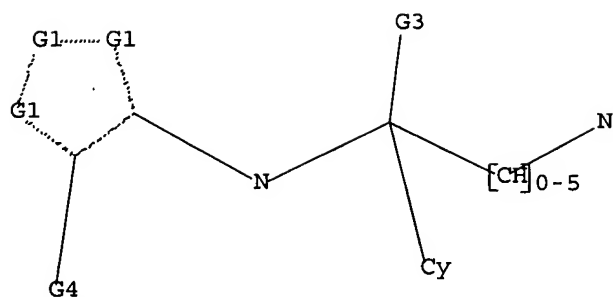
Number of Carbon Atoms : less than 7

L19 STRUCTURE UPLOADED

=> d

L19 HAS NO ANSWERS

L19 STR



G1 C, S

G2

G3 H, Me, Et, n-Pr, i-Pr, n-Bu, s-Bu

G4 X, MeO, EtO, n-PrO, i-PrO, n-BuO, s-BuO, CN, CHO, NH, NH2, NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l19

SAMPLE SEARCH INITIATED 14:03:32 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 45149 TO ITERATE

4.4% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 890294 TO 915666
PROJECTED ANSWERS: 0 TO 0

L20 0 SEA SSS SAM L19

=> s l19 full

FULL SEARCH INITIATED 14:03:40 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 909705 TO ITERATE

100.0% PROCESSED 909705 ITERATIONS
SEARCH TIME: 00.00.15

2 ANSWERS

L21 2 SEA SSS FUL L19

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

525.75

720.33

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-1.56

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FILE LAST UPDATED: 4 Sep 2007 (20070904/ED)

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=> s l21

L22 1 L21

=> d ibib abs hitstr tot

L22 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1984:191517 CAPLUS Full-text

DOCUMENT NUMBER: 100:191517

TITLE: Reactions of some arylmethylenedicarbamates with ethyl vinyl ether

AUTHOR(S): Sirotanovic-Maletic, Ksenija; Bajlon-Pastor, Milka; Markovic, Rade

CORPORATE SOURCE: Fac. Sci., Univ. Belgrade, Belgrade, YU-11001, Yugoslavia

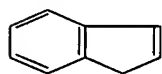
SOURCE: Glasnik Hemijskog Drustva Beograd (1983), 48(7), 401-8
CODEN: GHDBAX; ISSN: 0017-0941

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 100:191517

GI



N(CO₂Et)CHPhNHCO₂Et IV

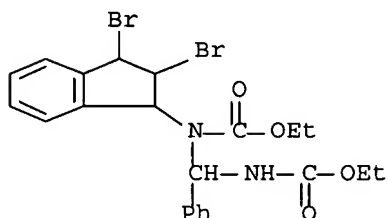
AB The title dicarbamates, RC₆H₄CH(NHCO₂R₁)₂ (I; R₁ = Et, R = H, 2-, 3-Cl, 2-, 4-MeO; R₁ = Me₂CHCH₂, R = H, 2-, 3-, 4- Cl), condense with EtOCH:CH₂ (II) in the presence of 1-2% BF₃.Et₂O (III) to give tricarbamates RC₆H₄CH(NHCO₂R₁)CH₂CH(NHCO₂R₁)₂. Electron-withdrawing substituents impede the reaction; I (R = NO₂) do not react under these conditions. With an excess of III present, I (R = H, R₁ = Et) reacted with II to give indan IV.

IT 89950-54-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

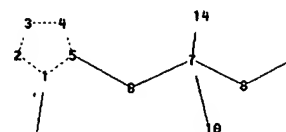
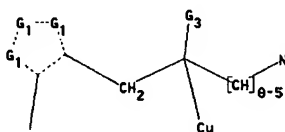
RN 89950-54-9 CAPLUS

CN Carbamic acid, (2,3-dibromo-2,3-dihydro-1H-inden-1-yl) [[(ethoxycarbonyl)amino]phenylmethyl]-, ethyl ester (9CI) (CA INDEX NAME)



=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728S-3str.str



chain nodes :

6 7 8 9 10 14 19

ring nodes :

1 2 3 4 5

chain bonds :

1-19 5-6 6-7 7-8 7-10 7-14 8-9

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-19 2-3 3-4 4-5 5-6 6-7 7-8 7-10 7-14 8-9

G1:C,S

G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom

14:CLASS 19:CLASS

Generic attributes :

10:

Saturation : Unsaturated

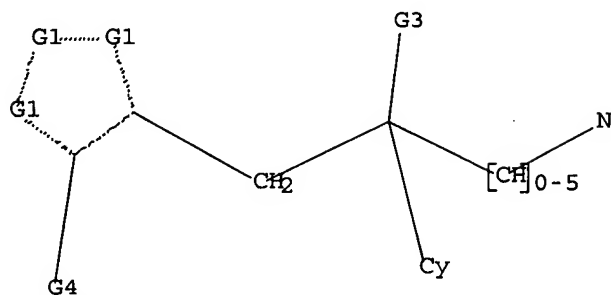
Number of Carbon Atoms : less than 7

L23 STRUCTURE UPLOADED

=> d

L23 HAS NO ANSWERS

L23 STR



G₁ C, S

G₂

G₃ H, Me, Et, n-Pr, i-Pr, n-Bu, s-Bu

G₄ X, MeO, EtO, n-PrO, i-PrO, n-BuO, s-BuO, CN, CHO, NH, NH₂, NO₂

Structure attributes must be viewed using STN Express query preparation.

=> s l23

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:05:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 44548 TO ITERATE

4.5% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 878358 TO 903562

PROJECTED ANSWERS: 0 TO 0

L24 0 SEA SSS SAM L23

L25 0 L24

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
0.47	727.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.34

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FILE LAST UPDATED: 4 Sep 2007 (20070904/ED)

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=> file reg
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
0.47	728.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.34

FILE 'REGISTRY' ENTERED AT 14:06:08 ON 05 SEP 2007
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STRUCTURE FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2
DICTIONARY FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

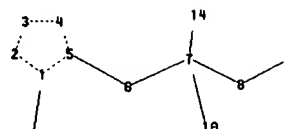
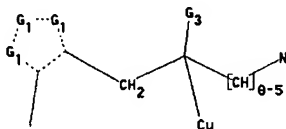
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728S-3str.str



chain nodes :

6 7 8 9 10 14 19

ring nodes :

1 2 3 4 5

chain bonds :

1-19 5-6 6-7 7-8 7-10 7-14 8-9

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-19 2-3 3-4 4-5 5-6 6-7 7-8 7-10 7-14 8-9

G1:C,S

G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom

14:CLASS 19:CLASS

Generic attributes :

10:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

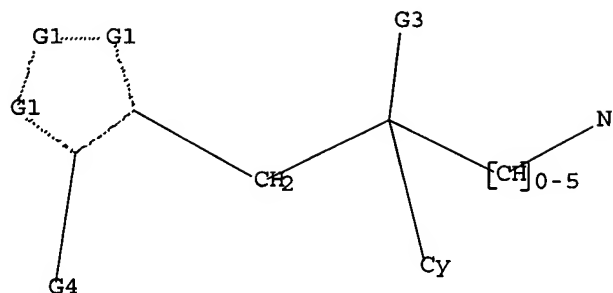
L26 STRUCTURE UPLOADED

=> d

L26 HAS NO ANSWERS

L26

STR



G1 C, S

G2

G3 H, Me, Et, n-Pr, i-Pr, n-Bu, s-Bu

G4 X, MeO, EtO, n-PrO, i-PrO, n-BuO, s-BuO, CN, CHO, NH, NH2, NO2

Structure attributes must be viewed using STN Express query preparation.

=> s 126

SAMPLE SEARCH INITIATED 14:06:39 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 44548 TO ITERATE

4.5% PROCESSED 2000 ITERATIONS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 878358 TO 903562
 PROJECTED ANSWERS: 0 TO 0

L27 0 SEA SSS SAM L26

=> s 126 full

FULL SEARCH INITIATED 14:06:46 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 894122 TO ITERATE

100.0% PROCESSED 894122 ITERATIONS
 SEARCH TIME: 00.00.10

0 ANSWERS

L28 0 SEA SSS FUL L26

=>

=>

Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS

SINCE FILE
 ENTRY

TOTAL
 SESSION

FULL ESTIMATED COST

173.00

901.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-2.34

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 14:07:47 ON 05 SEP 2007